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NEWS 1		Web Page for STN Seminar Schedule - N. America
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NEWS 3	MAR 16	CASREACT coverage extended
NEWS 4	MAR 20	MARPAT now updated daily
NEWS 5	MAR 22	LWPI reloaded
NEWS 6	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 7	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 8	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 10	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 11	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 12	MAY 01	New CAS web site launched
NEWS 13	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 14	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 15	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 16	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 17	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 18	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 19	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20	JUN 29	STN Viewer now available
NEWS 21	JUN 29	STN Express, Version 8.2, now available
NEWS 22	JUL 02	LEMBASE coverage updated
NEWS 23	JUL 02	LMEDLINE coverage updated
NEWS 24	JUL 02	SCISEARCH enhanced with complete author names
NEWS 25	JUL 02	CHEMCATS accession numbers revised
NEWS 26	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 27	JUL 16	CAplus enhanced with French and German abstracts
NEWS 28	JUL 18	CA/CAplus patent coverage enhanced
NEWS 29	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 30	JUL 30	USGENE now available on STN

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:22:19 ON 02 AUG 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:22:33 ON 02 AUG 2007
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DICTIONARY FILE UPDATES: 1 AUG 2007 HIGHEST RN 943895-11-2

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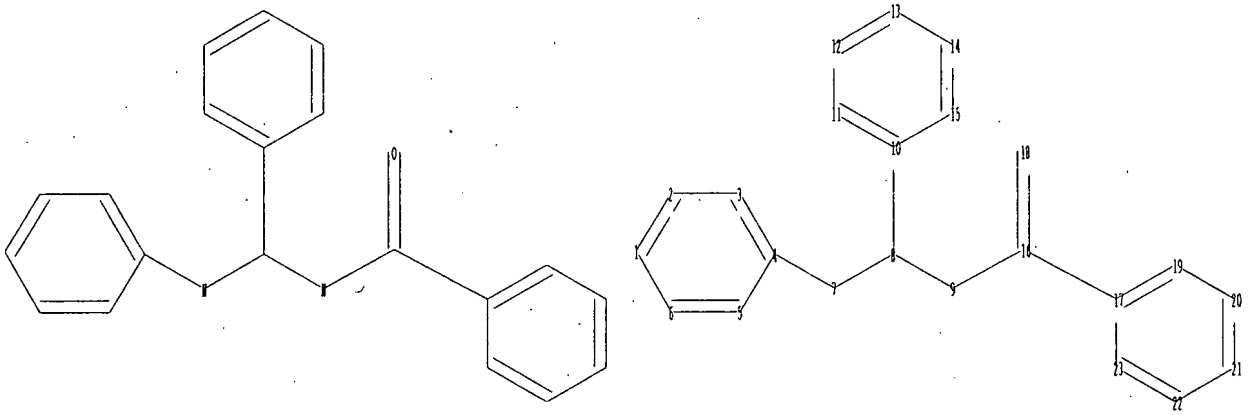
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10501932.str



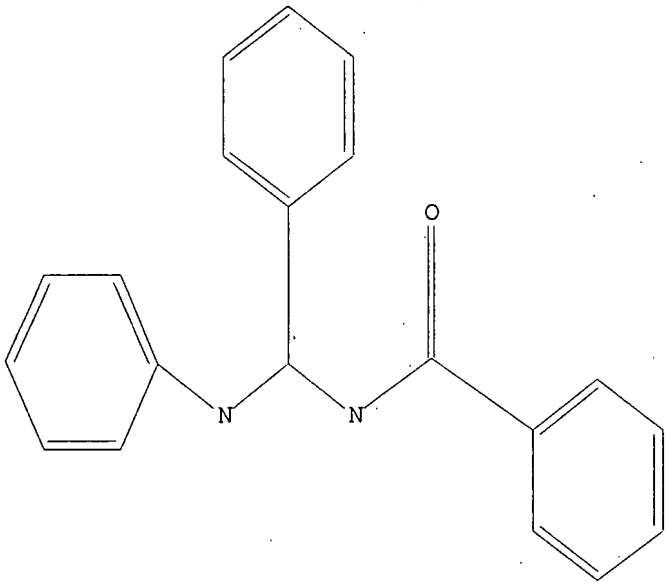
chain nodes :
7 8 9 16 18
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15 17 19 20 21 22 23
chain bonds :
4-7 7-8 8-9 8-10 9-16 16-17 16-18
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 17-19 17-23 19-20 20-21 21-22 22-23

exact/norm bonds :
4-7 7-8 8-9 9-16 16-18
exact bonds :
8-10 16-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 17-19
17-23 19-20 20-21 21-22 22-23

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:CLASS 19:Atom
20:Atom 21:Atom 22:Atom 23:Atom

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 14:22:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 28 TO ITERATE

100.0% PROCESSED 28 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 243 TO 877
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 14:22:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 513 TO ITERATE

100.0% PROCESSED 513 ITERATIONS 16 ANSWERS
SEARCH TIME: 00.00.01

L3 16 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 172.31

FILE 'CAPLUS' ENTERED AT 14:22:52 ON 02 AUG 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 2 Aug 2007 VOL 147 ISS 6
FILE LAST UPDATED: 1 Aug 2007 (20070801/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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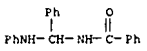
=> s l3
L4 15 L3

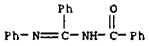
=> d ibib abs hitstr tot

L4 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:677988 CAPLUS
DOCUMENT NUMBER: 130:3816
TITLE: Monoacylaminals by the benzotriazole-assisted aminoalkylation of amides
AUTHOR(S): Katritzky, Alan R.; Fali, Clara N.; Bao, Weiliang; Qi, Ming
CORPORATE SOURCE: Center Heterocyclic Compounds, Department Chemistry, University Florida, Gainesville, FL, 32611, USA
SOURCE: Synthesis (1998), (10), 1421-1423
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:3816
AB A general synthesis of a range of monoacylaminals from the reaction of N-(α-aminoalkyl)benzotriazoles with amides in the presence of a base was developed. In less reactive cases ZnBr2 was used to facilitate the above reaction.
IT 215791-53-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of acylaminals by benzotriazole-assisted aminoalkylation of amides)
RN 215791-53-0 CAPLUS
CN Benzamide, N-[phenyl(phenylamino)methyl]- (9CI) (CA INDEX NAME)

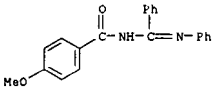


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

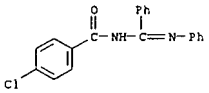
L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:5975 CAPLUS
DOCUMENT NUMBER: 114:5975
TITLE: Syntheses and structure of some acylamidines
AUTHOR(S): Marquez V., A.; Navarrete E., P. A.; Rodriguez C., H.; Pavez A., H.
CORPORATE SOURCE: Fac. Cienc. Quim. Farm., Univ. Chile, Santiago, Chile
SOURCE: Boletin de la Sociedad Chilena de Quimica (1989), 34(4), 269-77
CODEN: BOCQAX; ISSN: 0366-1644
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
AB N-Phenyl-N-acylbenzamidines and -acetamidines HN:NCRNPhCOR1 (R = Ph, Me; R1 = aryl) were prepared and shown to undergo thermal rearrangement to the N-phenyl-N1-acyl derivs. PhN:CRNHCOR1. Tautomers PhN:CMeNHCOC6H4NO2-p and PhNHCMe:NCOC6H4NO2-p were isolated and identified by spectroscopic methods.
IT 82208-28-4P 82208-29-5P 82208-30-8P
82208-31-9P 82208-32-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82208-28-4 CAPLUS
CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)



RN 82208-29-5 CAPLUS
CN Benzamide, 4-methoxy-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

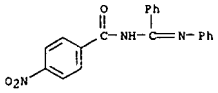


RN 82208-30-8 CAPLUS
CN Benzamide, 4-chloro-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

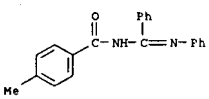


RN 82208-31-9 CAPLUS
CN Benzamide, 4-nitro-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

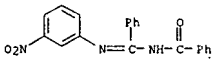
L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



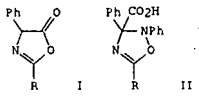
RN 82208-32-0 CAPLUS
CN Benzamide, 4-methyl-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:590788 CAPLUS
DOCUMENT NUMBER: 101:190788
TITLE: Reactions of derivatives of imidic acids with nucleophilic reagents. Kinetics of the reaction of N-substituted benzimidoyl chlorides with arylamines in aprotic media. Effect of amine structure
AUTHOR(S): Litvinenko, L. M.; Mikhailov, V. A.; Drizhd, L. P.; Savelova, V. A.; Kryuchkova, E. N.
CORPORATE SOURCE: Inst. Fiz.-Org. Khim. Uglekhim., Donetsk, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1984), 20(6), 1253-8
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Rate consts. were determined for aminolysis of PhCCl:NR (R = Me, Bz, SO2Ph) by
3-nitroaniline and some of its derivs. and by 4-nitroaniline. Hammett correlations with Σσ of the substituents in the anilines yielded ρ = -4.1 when R = SO2Ph and -2.2 when R = Me or Bz. A biomol. nucleophilic mechanism was proposed with transition states depending on R.
IT 92836-07-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 92836-07-2 CAPLUS
CN Benzamide, N-[[(3-nitrophenyl)amino]phenylmethylene]- (9CI) (CA INDEX NAME)

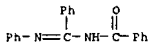


L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1983:198119 CAPLUS
DOCUMENT NUMBER: 98:198119
TITLE: Reaction between Δ2-oxazolin-5-ones and nitrosobenzene. Formation of 1,2,4-oxadiazolines
AUTHOR(S): Rodriguez, H.; Pavez, H.; Marquez, A.; Navarrete, P.
CORPORATE SOURCE: Fac. Cienc. Bas. Farm., Univ. Chile, Santiago, Chile
SOURCE: Tetrahedron (1983), 39(1), 23-7
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:198119
GI

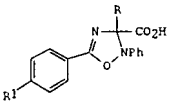


I II

AB Oxazolinones I (R = Ph, C6H4Me-4) reacted with PhNO at room temperature to give 59.5-90.7% oxadiazolines II, by regiospecific 1,3-dipolar cycloaddn. However, at 80-100°, PhC(:NPh)NHCOR (III) were formed. II decomposed to III on heating.
IT 82208-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by decomposition of oxadiazolinecarboxylate)
RN 82208-28-4 CAPLUS
CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

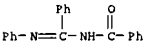


L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1982:423411 CAPLUS
DOCUMENT NUMBER: 97:23411
TITLE: Acylamidines
AUTHOR(S): Navarrete E., Patricio; Rodriguez C., Hernan; Pavez A., Hernan; Marquez V., Amelia
CORPORATE SOURCE: Fac. Cienc. Bas. Farm., Univ. Chile, Santiago, Chile
SOURCE: Boletin de la Sociedad Chilena de Quimica (1982), 27(2), 227-9
CODEN: BOCQAX; ISSN: 0366-1644
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
GI

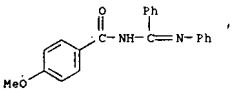


II

AB Acylation of HN:CPhNHPh with p-RC6H4COCl (R = H, MeO, Cl, NO2, Me) in CHCl3-Et3N at 0° gave 62-75% NH:CPhNPhCOC6H4R-p, which rearranged to PhN:CPhNHCOC6H4R-p (I) on brief heating in EtOH containing a strong acid (HCl, H2SO4). I were also obtained by heating oxadiazolines II in C6H6 or xylene.
IT 82208-28-4P 82208-29-5P 82208-30-8P
82208-31-9P 82208-32-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 82208-28-4 CAPLUS
CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

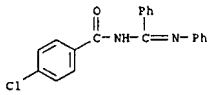


RN 82208-29-5 CAPLUS
CN Benzamide, 4-methoxy-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

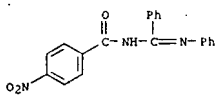


RN 82208-30-8 CAPLUS
CN Benzamide, 4-chloro-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

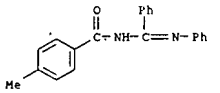
L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



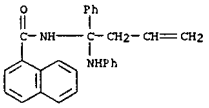
RN 82208-31-9 CAPLUS
CN Benzamide, 4-nitro-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)



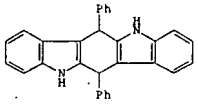
RN 82208-32-0 CAPLUS
CN Benzamide, 4-methyl-N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1978:190258 CAPLUS
DOCUMENT NUMBER: 88:190258
TITLE: The effect of crown ethers on the reductive dimerization of Schiff bases
AUTHOR(S): Smith, James G.; Chun, Ying-luen
CORPORATE SOURCE: Dep. Chem., Univ. Waterloo, Waterloo, ON, Can.
SOURCE: Tetrahedron Letters (1978), (5), 413-14
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 88:190258
AB In the reductive dimerization of N-benzalaniline by K in the presence of 18-crown-6 the complexation of the metal ion in solution imports addnl. stabilization to the reduced Schiff base PhCH:NPh•- enabling it to accept a second electron. The resulting dianion is relatively stable and was utilized in synthetic reactions such as alkylation with alkyl halides. Reaction with MeI, Br(CH2)3Br, and Cl(CH2)3Cl gave PhCHMeNMePh, PhCH(NHPh)CH2CH:CH2, and PhCPr:NPh, resp.
IT 66489-80-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66489-80-3 CAPLUS
CN 1-Naphthalenecarboxamide, N-[1-phenyl-1-(phenylamino)-3-butenyl]- (9CI) (CA INDEX NAME)

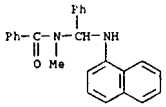


L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1977:453051 CAPLUS
DOCUMENT NUMBER: 87:53051
TITLE: Direct amidomethylation of heterocyclic amines
AUTHOR(S): Nelin, E. N.; Sheinkman, A. K.; Klyuev, N. A.; Marshtupa, V. P.; Khanetskii, A. B.
CORPORATE SOURCE: Donetsk. Gos. Univ., Donetsk, USSR
SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1977), 43(4), 391-7
CODEN: UKZHAU; ISSN: 0041-6045
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



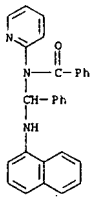
I

AB Reaction of BzCl, RCH:NR1 (R = Ph, 3-indolyl; R1 = Me, 2-naphthyl, 2-pyridyl, Ph) with amines, e.g., morpholine, 2,3-dihydroindole, 1,2,3,4-tetrahydroquinoline, 1-naphthylamine, and 2-pyridylamine gave 20-80% RCHR2NR1Bz (R2 = e.g., morpholino, 1-naphthylamino, 2-pyridylamino, 1,2,3,4-tetrahydro-1-quinolyl). Similar reaction of PhCH:NPh with indole gave I, which was identified by mass spectra.
IT 63232-82-6P 63232-86-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63232-82-6 CAPLUS
CN Benzamide, N-methyl-N-[(1-naphthalenylamino)phenylmethyl]- (9CI) (CA INDEX NAME)

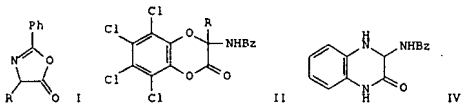


RN 63232-86-0 CAPLUS
CN Benzamide, N-[(1-naphthalenylamino)phenylmethyl]-N-2-pyridinyl- (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

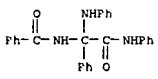


L4 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:523824 CAPLUS
DOCUMENT NUMBER: 85:123824
TITLE: o-Chloranil oxidation of azlactones
AUTHOR(S): Riordan, James M.; Stammer, C. H.
CORPORATE SOURCE: Dep. Chem., Univ. Georgia, Athens, GA, USA
SOURCE: Tetrahedron Letters (1976), (16), 1247-50
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 85:123824
GI

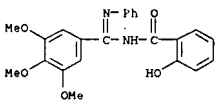


I II IV

AB Treatment of the azlactones I (R = PhCH2, Me2CH, Me, H, Ph, Me2CHCH2) with o-chloranil in Ac2O gave 60-95% benzodioxins II. II reacted with 2 equiv of MeO-, PhNH2, and PhCH2SH to give 60-85% BzNHCRR1CO2R1 (R1 = MeO, PhNH, PhCH2S, resp.). II (R = H) with EtOH gave BzNHCH(OC6H4OH-2)CO2Et (III); reaction of II (R = H) or III with o-H2NC6H4NH2 gave the tetrahydroquinoxaline IV.
IT 60422-74-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 60422-74-4 CAPLUS
CN Benzeneacetamide, α-(benzoylamino)-N-phenyl-α-(phenylamino)- (9CI) (CA INDEX NAME)

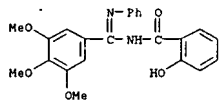


L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:82546 CAPLUS
DOCUMENT NUMBER: 62:82546
ORIGINAL REFERENCE NO.: 62:14669g-h
TITLE: The synthesis of 1,2-disubstituted 4-quinazolinones and related thiones
AUTHOR(S): Blatter, Herbert M.; Lukaszewski, Halina; de Stevens, George
CORPORATE SOURCE: CIBA Pharm. Co., Summit, NJ
SOURCE: Organic Chemistry (1965), 30(4), 1020-7
CODEN: OCSMBP; ISSN: 0078-611X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 62:82546
AB The Chapman rearrangement (imido esters to substituted amides) is applied to the synthesis of 1,2-disubstituted 4-quinazolinones. Addnl., the structure of the unusual acytation product of 2-methyl-1-phenyl-4-quinazoline is elucidated. The spectral characteristics of these compds. are discussed.
IT 1254-74-6P, Salicylamide, N-(3,4,5-trimethoxy-N-phenylbenzimidoyl)-
RL: PREP (Preparation)
(preparation of)
RN 1254-74-6 CAPLUS
CN Salicylamide, N-(3,4,5-trimethoxy-N-phenylbenzimidoyl)- (7CI, 8CI) (CA INDEX NAME)



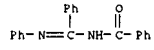
L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:82545 CAPLUS
DOCUMENT NUMBER: 62:82545
ORIGINAL REFERENCE NO.: 62:14668e-h,14669a-g
TITLE: The 1,5,8a,9-tetraazafluorene system. Synthesis of pyrido-[3',2':4,3]pyrazolo[1,5-a]pyrimidines
AUTHOR(S): Ried, Walter; Peuchert, Klaus Peter
CORPORATE SOURCE: Univ. Frankfurt/Main, Germany
SOURCE: Justus Liebigs Annalen der Chemie (1965), 682, 141-56
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 62:82545
GI For diagram(s), see printed CA Issue.
AB 2-Amino-5,7-dimethyl- (I), -5,6,7-trimethyl- (II), -5,7-dimethyl-6-ethyl- (III), and -7-methylpyrazolo-[1,5-a]pyrimidine (IV) condense with 1,3-dicarbonyl compds. under acid-catalyzed conditions to give 1,5,8a,9-tetraazafluorenes [pyrido[3',2':4,3]pyrazolo[1,5-a]pyrimidines] (V), whereas in neutral medium Schiff bases (VI) are formed. Condensation of I-III with cyclic 1,3-diketones of the type 2-acetylcyclohexanone (VII) gives 1,2,3,4 - tetrahydropyrimido [2',1': 5,1] pyrazolo-[3,4-c]isoquinolines (VIII). The properties of the new heterocyclic systems were described. I-III (0.005-0.01 mole) and a large excess 1,3-diketone (0.05-0.1 mole) [with BzCH2Ac (IX), some xylene was added] refluxed 3 hrs., the excess diketone evaporated in vacuo, and the residue recrystd. from EtOH gave the VI listed in the first table. I-III (0.01 mole) dissolved by heating in 0.05-0.1 mole 1,3-diketone, 3-5 drops concentrated HCl added, and the solution refluxed 15 min. and cooled gave V.HCl, which dissolved in a little H2O (if necessary with some EtOH) and treated with aqueous NaOH gave V.
amine, diketon, R, R1, R2, R3, R4, m.p.; I, Ac2CH2(X), Me, Me, H, Me, H, 134°; II, X, Me, Me, Me, Me, H , 165°; III, X, Me, Me, Et, Me, H, 149°; III, Ac2CHMe(XI), Me, Me, Et, Me, Me, 158°; III, IX, Ph, Me, Et, Me, H, 168°; The V listed in the second table were prepared Treatment of I-IV with β-oxocarboxylic acid esters (XV) as 1,3-dicarbonyl components also gave V, but in all these cases R5 = OH. I (1.62 g.) dissolved in 13 g. AcCH2CO2Et(XVI) by brief heating, 1-2 drops concentrated HCl added, and the solution refluxed 10 min. gave 1.9 g. V (R = R2 = R3 = Me, R1 = R4 = H, R5 = OH), decomposed 350° (DMF). amine, diketon, R, R1, R2, R3, R4, R5, m. p., decomposition point HCl salt, picrate; I, X, Me, H, Me, Me, H, Me(Xia), 180°, 338°, decomposition point picrate 222°; II, X, Me, Me, Me, Me, H, Me, 208°, 335°, 217°; III, X, Me, Et, Me, Me, H, Me, 166°, 292°, 225°; I, XI, Me, H, Me, Me, Me, Me, 257°, 295°, 224°; II, XI, Me, Me, Me, Me, Me, Me, 225°, 288°, 205°; III, XI, Me, Et, Me, Me, Me, Me, 168°, 286°, 223°; I, Ac2CHEt(XII), Me, H, Me, Me, Et, Me, 190°, 318°, 207°; II, XII, Me, Me, Me, Me, Et, Me, 204°, 322°, 202°; III, XII, Me, Et, Me, Me, Et, Me, 172°, 248°, 205°; I, IX, Me, H, Me, Me, H, Ph(XIIa), 205°, 303°, 256°; II, IX, Me, Me, Me, Me, H, Ph, 266°, 272°, 254°; III, IX, Me, Et, Me, Me, H, Ph, 183°, 245°, 217°; I, Bz2CH2(XIII), Me, H, Me, Ph, H, Ph (XIIIa), 227°, .., 240°; II, XIII, Me, Me, Me, Ph, H, Ph, 272°, .., 256°; III, XIII, Me, Et, Me, Ph, H, Ph, 215°, .., 248°; I, Bz2CHMe (XIV), Me, H, Me, Ph, Me, Ph, 217°, .., ..; II, XIV, Me, Me, Me, Ph, Me, Ph, 255°, .., ..;

L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
III, XIV, Me, Et, Me, Ph, Me, Ph, 207°, .., ..; The V (R5 = OH) listed in the third table were similarly prepd. XIa (2.3 g.) heated 10 min. at 220° with 2.2 g. 4-MeC6H4SO3Et (XX) and the melt cooled, dild. with 10 cc. EtOH, treated with 1.2 g. NH4ClO4, boiled 5 min., and cooled gave 2.7 g. perchlorate (XXI) of 1-Et deriv. of XIa, decompd. 175° (iso-PrOH). amine, XV, R, R1, R2, R3, R4, decompn. point; II, XVI, Me, Me, Me, Me, H, 390°(sulfate decompd.)285°); III, XVI, Me, Et, Me, Me, H, 348°; IV, XVI, H, H, Me, Me, H, 358°; I, AcCHMeCO2Et(XVII), Me, H, Me, Me, Me, 317°; II, XVII, Me, Me, Me, Me, Me, 360°; III, XVII, Me, Et, Me, Me, Me, 335°; IV, XVII, H, H, Me, Me, Me, 325°; I, AcCHEtCO2Et(XVIII), Me, H, Me, Me, Et, 352°; II, XVIII, Me, Me, Me, Me, Et, 390°; III, XVIII, Me, Et, Me, Me, Et, 346°; IV, XVIII, H, H, Me, Me, Et, 355°; I, BzCH2CO2Et(XIX), Me, H, Me, Ph, H, 320°; II, XIX, Me, Me, Me, Ph, H, 325°; III, XIX, Me, Et, Me, Ph, H, 332°; IV, XIX, H, H, Me, Ph, H, 322 °; From 0.58 g. XIIa and 0.5 g. XX and 0.7 g. XIIIa and 0.5 g. XX were similarly prepd. 0.4 g. perchlorate of 1-Et deriv. of XIIa, decompd. 245° (EtOH-EtOAc), and 0.6 g. perchlorate of 1-Et deriv. of XIIIa, decompd. 258° (DMF-H2O), resp. XXI (1.77 g.) in 5 cc. Ac2O boiled 10 min. with excess HC(OEt)3 and 5 drops Et3N and the mixt. dild. with H2O gave 0.8 g. XXII, decompd. 264° (DMF-EtOAc). I (1.62 g.) and 7 g. VII in 5 cc. xylene treated according to the general procedure for prepn. of V and the resulting HCl salt treated with 2N NaOH gave 1.2 g. VIII (R = R2 = R3 = Me, R1 = H), m. 196° (1:5 EtOH-H2O or ligroine); picrate decompd. 216° (EtOH). amine, cyclic 1,3-diketone, R, R1, R2, R3, m.p.; II, VII, Me, Me, Me, Me, 165°; III, VII, Me, Et, Me, Me, 170°; I, 2-propionylcyclohexanone(XXIII), Me, H, Me, Et, 171°(HCl salt decompd.262°); II, XXIII, Me, Me, Me, Et, 146°; III, XXIII, Me, Et, Me, Et, 153°; The VIII listed in the 4th table were prepd. similarly.
IT 1254-74-6P, Salicylamide, N-(3,4,5-trimethoxy-N-phenylbenzimidoyl)-
RL: PREP (Preparation)
(preparation of)
RN 1254-74-6 CAPLUS
CN Salicylamide, N-(3,4,5-trimethoxy-N-phenylbenzimidoyl)- (7CI, 8CI) (CA INDEX NAME)



L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:69121 CAPLUS
DOCUMENT NUMBER: 49:69121
ORIGINAL REFERENCE NO.: 49:13260h-i,13261a-e
TITLE: Analogs of Benadryl
AUTHOR(S): Blicke, F. F.; Toy, G. R.
CORPORATE SOURCE: Univ. of Michigan, Ann Arbor
SOURCE: Journal of the American Chemical Society (1954), 76, 4615-16
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The preparation is described of basic ethers of the general formula Ph2C(R)O(CH2)2X, where R is H, MeO, or Et2N(CH2)2O, and X is Et2N, morpholino, piperidino, 1-hexamethylenimino, or 4-methyl-1-hexamethylenimino. 2-(1-Hexamethylenimino)ethanol (I) (18.5 g.), 37.1 g. Ph2CHBr (II), and 16.6 g. K2CO3 heated 4 hrs. with stirring at 150-60° under N, the mixture cooled, diluted with 100 cc. H2O, and extracted with Et2O, the extract extracted with three 60-cc. portions 5% HCl, the acidic solution basified and extracted with Et2O, and the extract dried with K2CO3 and fractionated gave 22.3 g. benzhydryl 2-(1-hexamethylenimino)ethyl ether (III), b0.01 158-60°. III in Et2O treated with the calculated amount HCl in Et2O gave III.HCl, m. 144-6° (from dioxane); III in Et2O treated with excess MeBr deposited III.MeBr, m. 156-8° (from EtOAc-EtOH). 4-Me derivative of I (15.7 g.), 24.7 g. II, and 13.8 g. K2CO3 yielded similarly 18.7 g. 2-(4-methyl-1-hexamethylenimino) analog of III, b0.01 164-5°; HCl salt, m. 97-9° (decomposition) (from PhMe); methiodide, m. 189-90° (decomposition) (from absolute EtOH). (MeO)2CPh2 (IV) (56.7 g.) and HO(CH2)2Br heated 5 hrs. at 120-30° while distilling off 6.6 g. MeOH and the residue fractionated gave 47.0 g. Ph2C(OMe)O(CH2)2Br (V), b3 169-70°. III (35.7 g.), 94.6 g. piperidine, and 50 cc. C6H6 heated 5 days in a pressure bottle at 60° the mixture washed with 20% aqueous NaOH and then with H2O, and the C6H6 layer distilled gave 36% α-methoxybenzhydryl β'-piperidinoethyl ether (VI), b. 145-7°; HCl salt, m. 179-80° (decomposition) (from CHCl3-Et2O). III (35.7 g.), 50 cc. C6H6, and 96.9 g. morpholine yielded similarly 11.5 g. 2-morpholinoethyl analog of VI, b0.01 153-6°; HCl salt, m. 162-3° (decomposition). IV (22.8 g.) and 25.5 g. Br(CH2)2OH heated 24 hrs. at 135° while distilling off 4.9 g. MeOH, the unreacted Br(CH2)2OH distilled off, the residual oil heated 3 days at 60° in a pressure bottle with 54.9 g. Et2NH in 50 cc. C6H6, the mixture treated with 10 g. NaOH in 25 cc. H2O, and the organic layer washed with H2O and fractionated gave 12.7 g. (Et2NCH2CH2O)2CPh2, b0.05 148-50°; di-HCl salt, m. 148-9° (decomposition) (from CHCl3-Et2O). α-Methyl-α-phenyl-2-pyridinemethanol (VII) (24.0 g.) in 150 cc. PhMe treated with 2.7 g. Na, and the mixture treated with the chloride obtained by the addition of 11.2 g. KOH, 100 cc. H2O, and 150 cc. PhMe to 27.8 g. 2-(1-hexamethylenimino)ethyl chloride HCl salt (VIII) yielded 22.5 g. α-phenyl-α-(2-pyridyl)-β'-(1-hexamethylenimino)diethyl ether (IX), b0.05 164-5°; methobromide, m. 222-4° (decomposition) (from EtOH). VII (24.0 g.), 2.7 g. Na, 34.0 g. 4-Me derivative of VIII, and 300 cc. PhMe gave similarly 25.8 g. β'-(4-methyl-1-hexamethylenimino) analog of IX, b0.05 157-9°; HCl salt, m. 143-5° (decomposition) (from EtAc).
IT 82208-28-4P, Benzamide, N-(N-phenylbenzimidoyl)-
RL: PREP (Preparation)
(preparation of)
RN 82208-28-4 CAPLUS
CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:69120 CAPLUS
DOCUMENT NUMBER: 49:69120
ORIGINAL REFERENCE NO.: 49:13259i,13260a-h
TITLE: Cyclic amidines. I. Derivatives of phenhomazine (dibenzo[b,f]-1,5-diazocine)
AUTHOR(S): Cooper, F. C.; Partridge, M. W.
CORPORATE SOURCE: Univ. Nottingham, UK
SOURCE: Journal of the Chemical Society (1954) 3429-35
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

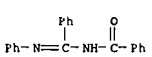
AB -2-NCC6H4NH2.p-HO3SC6H4Me (I), on heating, forms 6,12-diaminophenhomazine (II) and tricycloquinazoline (III). Dianthranilide (IV) was prepared by interaction of Me anthranilate (V), a nitrile, and Na. This reaction was applicable to a number of analogous reactions. The light absorption characteristics of a number of phenhomazine derivs. are given. o-ClC6H4NO2 (52.5 g.), 32.9 g. Cu2 (CN)2, and 29 g. C5H5N heated 4 hrs. at 160°, then 1 hr. at 180°, and the mixture added to 350 ml. HCl gave 32 g. o-NCC6H4NO2, m. 107.5-8.5° (from HOAc). o-NCC6H4NH2 heated with 25 g. p-MeC6H4SO3H in H2O gave 27.7 g. I, prisms, m. 170-1°; picrate, red prisms, m. 109-10° (from H2O). I (20 g.) heated 15 min. in a refluxing PhNO2-vapor bath, and the cooled melt extracted with H2O and 1.5N HCl yielded 1.9 g. III, needles, m. 322-3°; the aqueous extract yielded 0.25 g. of the p-toluenesulfonate of II, orange needles, m. 280-2°; monopicrate, m. 225-7°. Another p-toluenesulfonate (0.95 g.), m. 228-9°, separated during this purification but was not identified. The aqueous filtrate and acid extract combined, made alkaline with NH3, and the precipitate crystallized from 4N HCl yielded 2.55 g. II.2HCl.H2O, m. 285-7°. o-H2NC6H4CHO (4 g.) and 10 g. NH4Cl treated by the method of Kozak and Kalmus (C.A. 28, 4424.3) gave 0.6 g. III (from PhMe). Indazole (1 g.) and Cu powder heated as described by Jacobson and Huber (C.A. 2, 1566), gave 0.15 g. III, whose ultraviolet absorption spectrum showed peaks at 252, 284, 296, 310, 378, 400, 424, and 452 mμ. When 45.4 g. V, 13.8 g. Na, and 24.6 g. MeCN (VI) were mixed with C6H6 at room temperature, an initial exothermic reaction caused boiling; the mixture refluxed 24 hrs., the product shaken with H2O and 2N NaOH, and the aqueous solns. charcoaled and treated with excess HCl afforded 17.1 g. crude IV; crystallization from EtOH gave pure IV, m. 335-7°. With 0, 0.5, and 21 hrs. of refluxing, the yields of IV were 30, 31, and 40%, resp.; with twice the amount of VI and 3.5 hrs. refluxing, 38%; with twice the amount of VI and Na and 20 hrs. refluxing, 44%. After removal of the IV, the mother liquors afforded 0.4 g. of a compound which may have been 2-anthraniloylmethyl-4-hydroxyquinazoline, yellow needles, m. 176-7°. V (22.7 g.), 6.9 g. Na, and 30.9 g. PhCN (VII) heated in C6H6 reacted vigorously; the mixture refluxed 2 hrs. and similarly treated gave 8.8 g. IV. Neutralization of the filtrate with NH3 gave 1.5 g. 4-hydroxy-2-phenylquinazoline, m. 235-6°. Distillation of the extracted C6H6 solution gave 7.25 g. VII. Repetition of this reaction with 0.23 mole VII and refluxing 3 and 4 hrs. gave 55 and 56% yields of IV, resp. V (0.1 mole) and 0.1 g. atom of Na refluxed 8 hrs. in C6H6 gave 4% IV, while 12 hrs. in refluxing EtOH gave 3% IV. No IV was obtained when V, Na, EtOH, and C6H6 were refluxed 22 hrs. N,N'-Bis(p-toluenesulfonyl)dianthranilide, an intermediate, m. 252-3°, rising on storage to 271-2°. 6,12-Dichlorophenhomazine (VIII), m. 219-20°, and N,N'-dimethyldianthranilide, m. 205-7°, were prepared by Schroeter and Eisleb's method (C.A. 3, 2976). IV shaken with Et2SO4 in 0.5N NaOH 6

L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
hrs. gave 60% of the N,N'-di-Et deriv., prisms, m. 192-3°. VIII (2 g.) refluxed 26 hrs. with Na in MeOH yielded 1.8 g. 6,12-dimethoxyphenhomazine, prisms, m. 161-2°; monopicrate, prisms, m. 144-55°. VIII similarly forms 98% 6,12-di-EtO deriv., m. 146-7°. VIII (5 g.) in 14% w./w. MeOH-NH3 heated 6 hrs. at 120-50°, the residue treated with 1.5N HCl, and 0.4 of this soln. neutralized with NH4 afforded 1.7 g. II, cubes, m. 127-8° (from aq. MeOH), rods, m. 92-3° (effervescence) (from C6H6). The remaining 0.6 of the acid soln. yielded 3.2 g. (54%) II.2HCl, m. 283-6° (decompn.); crystd. from 4N HCl, it m. 285-7° (decompn.). The di-HCl salt with hot H2O gave the mono-HCl, salt, m. 283-7°; monopicrate, m. 227-8° (decompn.). VIII treated with EtOH-NH3 3 weeks at room temp. or with NaNH2 or heated at 120-30° with (NH4)2CO3 in PhOH or at 210° with urea for 22 hrs. reflux gave no recognizable basic products. Na N-phenylbenzamidine (IX) [from 9.8 g. PhC(:NH)NHPh] refluxed 8 hrs. with 7.5 g. BzOEt in C6H6 yielded 0.9 g. BzOH, 0.4 g. Bz2NH, and 2.7 g. unchanged IX. BzNHPh (0.15 g.) and 3.4 g. PhC(:NPh)NHBz were isolated from the C6H6-insol. products.

IT 82208-28-4P, Benzamide, N-(N-phenylbenzimidoyl)-
RL: PREP (Preparation)
(preparation of)

RN 82208-28-4 CAPLUS

CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1953:12057 CAPLUS
DOCUMENT NUMBER: 47:12057
ORIGINAL REFERENCE NO.: 47:2134f-i,2135a-i,2136a
TITLE: Diamidides. II. 2,4-Diaryltriazapentadienes
AUTHOR(S): Peak, D. A.
CORPORATE SOURCE: Boots Pure Drug Co., Ltd., Nottingham, UK
SOURCE: Journal of the Chemical Society (1952) 215-26
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 47:12057

AB cf. C.A. 46, 1985d. A general method for the preparation of N'-thiobenzoylbenzamidines, PhCSN:CArNH2, has been developed; they are shown to undergo fission by NH3 or primary amines, mainly by reaction at the amidine-C atom. When benzamidines are used instead of amines, the reaction gives rise to 2,4-diaryltriazapentadienes, H2NCAr:NCAr':NH, isolated as their relatively stable hydrated HCl salts. PhC(:NH)NHBz also undergoes fission but considerably more slowly than its thio analog. The rate of reaction is much increased by a Ph group as in PhC(:NBz)NHPh, although side reactions occur. PhC(:NH)NPhBz also reacts rapidly but probably by a different mechanism. 2,4-(O2N)2C6H3NHC(:NH)Ph reacts abnormally, whereas p-HO3SC6H4NHC(:NH)Ph is quite stable to NH3. The mechanisms of these reactions are discussed. p-MeOC6H4C(:NH)NH2.HCl (28 g.), shaken with 28 cc. H2O, 56 cc. 5 N NaOH, and 80 cc. CHCl3, the aqueous layer extracted with three 80-cc. portions of CHCl3, and the solution [290 cc. containing 19.13 g. p-MeOC6H4C(:NH)NH2] and 25.25 g. BzOPh kept overnight, give 19.2 g. N-benzoyl-p-methoxybenzamidine (I), m. 104-5°. p-ClC6H4C(:NH)NH2.PhSO3H (3.13 g.) gives 1.4 g. N-benzoyl-p-chlorobenzamidine (II), m. 121-2°. p-MeSO2C6H4C(:NH)NH2 (10.7 g.) and 10 g. BzOPh, heated 6 hrs. at 70-5°, give 1.2 g. N-benzoyl-p-(methylsulfonyl)benzamidine (III), m. 223-4°. 2,4-(O2N)2C6H3CO2H (27.2 g.), 12 g. PhOH, and 27.2 g. POCl3, heated 40 min. at 115°, give 15.7 g. Ph 2,4-dinitrobenzoate (IV), m. 82-3°. PhC(:NH)NH2 (4.8 g.) and 11.5 g. IV in 160 cc. CHCl3, with final heating 3 hrs. at 60° in the absence of CHCl3, and the deep purple product in 50 cc. Me2CO acidified with 5 N EtOH-HCl, give the HCl salt, m. 194-6°, of N-(2,4-dinitrobenzoyl)benzamidine, pale yellow, m. 108-10° to a deep red liquid. PhCSNH2 (10.28 g.) and 7.73 g. PhCN in 350 cc. ether, saturated at 0° with dry HCl and kept 5 days at room temperature, give 59.5% PhCSN:C(Ph)NH2 (V). Substituted thiobenzamides and PhCN did not react because of the almost complete precipitation of the thioamide as the HCl salt; ether could not be replaced by dioxane or CHCl3 and the condensation also failed in anhydrous HF. PhC(:NH)NHBz.HCl (2.2 g.) and 2.4 g. PCl5 in 10 cc. CHCl3 refluxed 15 min., and the yellow oil in 10 cc. (CHCl3 added dropwise to 1.7 g. Et3N in 20 cc. CHCl3, saturated at 0° with dry H2S, and treated 3 hrs. with H2S give 25% V; in the same way I yields 48.5% p-methoxy-N-(thiobenzoyl)benzamidine (VA), red, m. 116-17°; II gives 26% p-chloro-N-(thiobenzoyl)benzamidine (VB), red, m. 146-7°. The HCl salt of III (2.03 g.) reacts partially with PCl5 in CHCl3; after 30 min., it yields 0.36 g. p'-(methylsulfonyl)benzanilide, m. 171-2°; the CHCl3 solution, treated with Et3N saturated with H2S, gives 0.6 g. p-(methylsulfonyl)thiobenzamide (VI), pale yellow, m. 217-18° (decomposition), and 0.19 g. PhCSNH2. p-MeSO2C6H4CN (0.9 g.) in 15 cc. CHCl3 and 1.5 cc. Et3N, saturated at 0° with HgS and kept 6 hrs., gives 0.96 g. VI. V (0.48 g.), 1.81 g. HgO, 1 g. PhNH2, and 10 cc. EtOH, shaken about 1 hr., give 0.4 g. H2NCPh:NCPh:NPh. V (0.12 g.) in 3 cc. 2 N absolute EtOH-NH (30 min.), gives

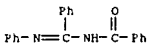
L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
88% PhCSNH2 and 74% PhC(:NH)NH2 (isolated as the picrate); in the presence of HgO, HgCl2.NH4Cl, or Pb(OH)2, there were isolated in addn. cyaphenine (2,4,6-triphenyl-s-triazine) (VIA), 3,5-diphenyl-1,2,4-thiadiazole (VII), and a picrate, C20H20N4S.C6H3O7N3, yellow, m. 187-8°. V (3.84 g.) and 1.71 g. PhCH2NH2 in 40 cc. ether, kept a few hrs., give 78% PhC(:NH)NHCH2Ph (as the picrate) and 0.19 g. PhC(:NH)NH2 (as the picrate); the original ether layer gives 58.5% PhCSNH2 and 0.12 g. PhCSNHCH2Ph. V (4.8 g.) and 2.4 g. PhC(:NH)NH2 in 95 cc. ether, kept overnight, give 1.52 g. VIA; the filtrate, acidified with 5 N EtOH-HCl, gives 3.55 g. of a solid (VIII); the filtrate yields 1 g. PhCSNH2. VIII, extd. with H2O and the residue (2.81 g.) treated in 40 cc. abs. EtOH with 80 cc. Me2CO, gives 2.16 g. 2,4-diphenyl-1,3,5-triaza-1,3-pentadiene-HCl (VIIIA), with 0.5 mol. H2O, m. 204-6° (picrate, yellow, m. 188°, clears 230°); sublimation at 200°/2 mm. gives VIA; the free base of VIIIA is an oil which gradually deposits VIA. VA (1 g.) and 0.56 g. p-MeOC6H4C(:NH)NH2 in 250 cc. ether, kept 40 hrs., give 0.62 g. of 2,4-bis(p-methoxyphenyl)1,3,5-triaza-1,3-pentadiene-HCl, with 1 mol. H2O, m. 176-8°; 2,4-bis(p-chlorophenyl) analog, with 0.5 mol. H2O, m. 220-1°. PhC(:NH)NH2 (0.44 g.) and 1 g. VA in 25 cc. ether, kept 24 hrs. and the filtrate acidified with 5 N EtOH-HCl, give 0.115 g. 2-(p-methoxyphenyl)-4-phenyl-1,3,5-triaza-1,3-pentadiene, m. 163-5° (slow heating). V (0.96 g.) and 0.76 g. PhC(:NH)NHPh in 8 cc. C6H6, refluxed 60 hrs., give 0.45 g. VIA and 20 mg. PhNHCPh:NCPh:NPh. PhC(:NH)NHBz (IX) (0.5 g.) in 5 cc. EtOH, refluxed 24 hrs., gives 0.1 g. VIA, 0.21 g. unchanged IX, and a little BzOEt. IX (0.5 g.) and 5 cc. 2 N EtOH-NH3, kept 7 days at room temp. and the residue in 2 cc. 2 N HCl basified, give 0.27 g. IX and, on addn. of picric acid to the mother liquor, 0.13 g. PhC(:NH)NH2 [as the picrate (X)]. IX (0.9 g.) and 0.43 g. PhCH2NH2 in 10 cc. abs. EtOH, kept 7 days at room temp., give 0.03 g. BzNH2, 0.02 g. BzNHCH2Ph, and 0.71 g. (40.5%) PhC(:NH)NHCH2Ph (as the picrate) and 0.03 g. X. IX (4.5 g.) and 1.9 g. PhNH2, heated 2 hrs. at 180° and the product extd. with ether, give 2.41 g. insol. material (0.52 g. VIA and 1.75 g. BzNH2); the residue from the ether (1.52 g.), extd. with N HCl, gives 3% PhNHBz, 5.5% PhC(:NPh)NHPh.HCl, and 7.5% PhC(:NH)NHPh. PhC(:NH)NHPh (9.8 g.) in 100 cc. CHCl3 and 6.06 g. Et3N at 0-1°, treated with 7.03 g. BzCl, give 5.55 g. PhC(:NH)NBzPh (XI); crystn. of XI from EtOH gives PhC(:NBz)NHPh (XII), m. 110°. XII and alc. NH3 (24 hrs.) give 19% BzNH2, 32% PhC(:NH)NHBz, and 30% PhC(:NH)NHPh. XII and PhCH2NH2 in ether, refluxed 12 hrs., give 55.5% PhC(:NBz)NHCH2Ph and 17% PhC(:NH)NHPh. XI and 2 N EtOH-NH3 give 68% BzNHPh, 2% PhC(:NH)NH2, and 5% PhC(:NH)NHPh. PhC(:NH)NHPh (4.2 g.) in 100 cc. ether, treated with 3.01 g. BzCl and shaken 1 hr., give 1.06 g. N,N'-dibenzoyl-N-phenylbenzamidine (XIII), m. 141-2°; 0.5 g. XIII in 5 N HCl and 5 cc. EtOH, shaken overnight, give 0.13 g. BzNHPh and 0.1 g. Bz2NH; 0.5 g. XIII in 10 cc. 2 N EtOH-NH3, shaken 90 min. and kept overnight, give 0.13 g. BzNHPh and 0.1 g. PhC(:NH)NHBz (as the picrate). PhC(:NH)NHSO2Ph does not react with 2 N EtOH-NH3. PhC(:NH)NH2 and PhC(:NH)OEt, heated 24 hrs. at 100°, give some VIA and 2.6% XIIA; the reactants, refluxed 3 days in C6H6. Give 1.05% XIIA. PhC(:NH) NH2 in C6H6, refluxed 3 days, give 0.35% XIIA.

IT 82208-28-4P, Benzamide, N-(α-anilinobenzylidene)-
RL: PREP (Preparation)
(preparation of)

RN 82208-28-4 CAPLUS

CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)

L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1952:11293 CAPLUS
DOCUMENT NUMBER: 46:11293
ORIGINAL REFERENCE NO.: 46:1985d-i,1986a-h
TITLE: Diamidides. I. Derivatives of triazapentadiene and tetraazaheptatriene
AUTHOR(S): Cooper, F. C.; Partridge, M. W.; Short, W. F.
CORPORATE SOURCE: Boots Pure Drug Co. Ltd., Nottingham, UK
SOURCE: Journal of the Chemical Society (1951) 391-404
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB PhCN (2 mols.) and PhSO3NH3Ph, heated 1 hr. at 200-20°, give 91% PhC(:NH)NHPh (I); it is unlikely that a diamide, NR:CPhNR'CPh:NR'' or RR'NCPh:NCPh:NR'', is present. I and p-NCC6H4SO2Me are unchanged after heating 4 hrs. at 180°. PhC(:NH)NH2 and PhN:CPhCl (II) in ether (90 min.), give 72% PhN:CPhN:CPhNH2 (III), m. 146-7°; picrate, with 0.5 mol. H2O, m. 167-8°; benzenesulfonate, m. 207-7.5°; heated 1 hr. at 190-200°, III yields PhCN and 83% I. II (4.3 g.) in 30 cc. ether, treated with 6.6 g. m-O2NC6H4C(:NH)NH2, shaken 1 day, the residue extracted with 20 cc. hot H2O, and the product in hot EtOH acidified with dilute HCl, give 41% 4-(m-nitrophenyl)-1,2-diphenyl-1 3,5-triaza-1,3-pentadiene (IV) as the HCl salt, m. 219-21° (decomposition); boiled in C6H6 1 hr., the reactants give 47% IV. II (4.3 g.) and 8.4 g. PhC(:NH)NMePh in 90 cc. C6H6, kept 11 days, give 82% 5-methyl-1,2,4,5-tetraphenyl-1,3,5-triaza-1,3-pentadiene (IVA), yellow, m. 104.5-5°; HCl salt, m. 234-4.5°; picrate, orange yellow, m. 159.5-60.5°; equimol. quantities of reactants in 15 mols. C5H5N give 17% IVA. 1,2,4,5-Tetraphenyl-1,3,5-triaza-1,3-pentadiene (V) (1.9 g.) and 0.205 g. NaNH2 in 50 cc. C6H6, heated 2.5 hrs., treated with 1.4 g. MeI in 10 cc. C6H6, and boiled 90 min., give 39% unchanged V and 36% IVA; V is not methylated by MeI in the presence of K2CO3 or by heating with a large excess of MeI 17 hrs. at 100°. PhC(:NH)NHBz (preparation in 68-78% given) (7.5 g.) and 5.45 g. PCl5 in dry CHCl3, treated with 9.4 g. PhNHMe, kept 90 min., boiled 90 min., and extracted with H2O, gives 43% IVA and, from the aqueous extract, 5% of the HCl salt. MeN:CPhCl (VI) (3.1 g.) and PhC(:NPh)NHPh (VII) (10.9 g.) in 150 cc. C6H6, kept 9 days, give 81% 1-methyl-2,3,4,5-tetraphenyl-1,3,5-triaza-1,4-pentadiene (VIII), pale yellow, m. 148.5-9.5°, and 41% recovery of VII; with equimol. quantities of VI and VII, the yield (after 1 day in C5H5N) is 73%; in Me2CO containing K2CO3, 98% of VII is recovered. II (4.3 g.) and 8.4 g. PhC(:NPh)NHMe (IX) in 300 cc. C6H6, kept 9 days, give 94% VIII. VIII in aqueous EtOH, lactic acid, and Na picrate give a mixture of the picrates of VII (44%) and IX (14%). III (5.4 g.) and 13.6 g. VII in 200 cc. C6H6, kept 13 days, gives 7.2 g. unchanged VII (as HCl salt) and 79% 1,2,3,4,5-pentaphenyl-1,3,5-triaza-1,4-pentadiene, pale yellow, m. 149-50°. II (2.7 g.) and 6.8 g. PhC(:NH)NPh2 in C6H6, kept 12 days, give 92% 1,2,4,5,5-pentaphenyl-1,3,5-triaza-1,3-pentadiene, m. 137.5-8°; picrate, yellow, m. 167-8°. PhC(:NPh)NHBz (7.5 g.) and 5.2 g. SOCl2 in 40 cc. CHCl3, kept 5 days at 20°, heated 2 hrs. at 100°, treated with 6.4 g. p-ClC6H4NH2 in 30 cc. C6H6, and kept 4 days, give 10% 1-p-chlorophenyl-2,4,5-triphenyl-1,3,5-triaza-1,3-pentadiene, pale yellow, m. 177-9°. PhC(:NPh)NHBz (7.5 g.) and 5.2 g. PCl5 in 40 cc. CHCl3 (exothermic reaction), kept 1 day, give 26% of a compound C20H15N2Cl, gradually decomps. above 160°; 1 g. and 5 g. PhNH2 in 30 cc. C6H6, kept 6 days, give 30% V, pale yellow, m. 183.5-4°; HCl salt, m. 250-4° (decomposition) and then

L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

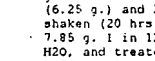
300-6°; picrate, yellow, m. 190-1°. PhC(:NPh)NHBz (6.85 g.), 5 g. PCl5, and 2.35 g. PhNH2 in C6H6, refluxed 4 hrs., give 12% I; 7.5 g. PhC(:NPh)NHBz and 5.45 g. PCl5 in 50 cc. CHCl3, kept 1 hr. at 20°, treated with 8.2 g. PhNH2 in 50 cc. CHCl3, and kept 6 days, give 54% PhCN and 17% V; in C5H5N, the yield of V is 5%. PhC(:NPh)NHBz (6.25 g.) and 3.8 g. PCl5 in 150 cc. C6H6, boiled 90 min., concd., and shaken (20 hrs.) with EtOH-NH3, give 61% PhC(:NPh)NHPh. II (4.3 g.) and 7.85 g. I in 120 cc. C6H6, kept 5 days, evapd., extd. with 50 cc. warm H2O, and treated with NH4OH, give 79% I; the H2O-insol. portion, sepd. by cold aq. lactic acid, gives 62% PhC(:NPh)NHPh and 6% V; after 1 day the yield of V was 3%; in 1 expt. in which the time was 4 days, the basic material, sparingly sol. in lactic acid, yielded 5% V and 7% 1,2,4,5,6,7-hexaphenyl-1,3,5,7-tetraaza-1,3,6-heptatriene (X), yellow, m. 178.5-9.5°. I and II in ether (2 days) give 17% X; in alc.-free CHCl3, the products included 16% V and 9% X; with K2CO3 in Me2CO, boiled 2 hrs., 16% X is formed. PhZCNOSO2Ph (27 g.) and 31.4 g. I in 300 cc. CHCl3, refluxed 30 min., give 22% V. BzNHPh (4.9 g.) and 4.5 g. PhSO2Cl in 6 cc. C5H5N, heated 90 min. at 100°, treated with 9.5 g. I in 8 cc. C5H5N, and heated an addnl. 3 hrs., give 23% V (17% after 90 min.). PhC(:NPh)NHBz (7.5 g.), 4.4 g. PhSO2Cl, and 6 g. anhyd. C5H5N, heated 2.5 hrs. at 100°, treated with 4.65 g. PhNH2, heated 90 min., kept overnight, poured into 250 cc. H2O and 15 cc. concd. HCl, give 3.1 g. PhC(:NPh)NHPh, 7% BzNHCH2Ph, 31% PhCN, and 32% I. PhC(:NPh)NHBz (7.5 g.) and 4.4 g. PhSO2Cl in 6 g. anhyd. C5H5N, heated 2.5 hrs. at 100° and poured into 100 cc. H2O and 15 cc. concd. HCl, give 54% BzNHPh, 28% PhCN, 1.6% V, and 77% PhSO3H. IV (1 g.), heated 1 hr. at 190-200°, gives 0.9 g. IV, m. 182.5-3.5°. IV (1.9 g.), 2.5 g. PhSO2NH3Ph, and 1.6 g. C5H5N, heated 90 min. at 100°, poured into 100 cc. H2O, and acidified with HCl, give 90% PhC(:NPh)NHPh. IV (1.9 g.) is not completely dissolved when heated at 100° with 0.95 g. PhNH2; 84% IV is recovered; 1.9 g. IV, 0.95 g. PhNH2, and 1.2 g. C5H5N, heated 90 min. at 100°, give on acidification 90% IV. IV (1.9 g.), 1.2 g. PhSO3H.C5H5N, and 1.6 g. C5H5N, heated 90 min. at 100°, give 92% unchanged IV. IV (1.9 g.), 65 cc. (CH2OH)2, 3 cc. H2O, and 4 g. KOH, boiled 3 hrs., give 74% BzOH; 1.9 g. IV and 4 g. KOH in 4 cc. H2O and 20 cc. EtOH, boiled 25 hrs., give 76% IV and 15% I. IX in EtOH, treated with HCl and dild. with H2O, gives 25% BzNHPh, 46% X, and 25% IX; in CHCl3, HCl yields 91% BzNHPh and 86% X. IX (15 g.) in 250 cc. C6H6, satd. with dry HCl, the C6H6 evapd., the residue treated with p-ClC6H4NH2, and kept 4 hrs., give 14% IX and 17% p-ClC6H4NH3Cl; the pptd. oil, freed from HCl at 0.5 mm. and the gum (15 g.) in 200 cc. C6H6 contg. 4.6 g. p-ClC6H4NH2 kept 5 days, give 11.25 g. of a ppt.; the H2O-sol. fraction yields 30% PhC(:NMe)NHPh, m. 131-3°; the H2O-insol. portion yields 5% BzNHPh and 7% N-p-chloro-phenyl-N'-methylbenzimidine (XI), m. 129-30° (picrate, m. 179-80°) (synthesis given). PhC(:NH)NHMe (2.25 g.) and 2.4 g. SOCl2 heated 1 hr. at 100°, treated with 4.25 g. p-ClC6H4NH2, and kept 4 days, give 63% XI. PhC(:NPh)NHBz (7.5 g.) and 5.45 g. PCl5 in 50 cc. CHCl3, shaken 4 hrs., added dropwise at 0° to 23 g. PhC(:NPh)NHPh give 7% X; the lactic acid-sol. fraction yields 9% V; 4.3 g. II in anhyd. ether, added slowly to 7.85 g. I in MeOH and kept 3 days, gives 23% X and 21% V. X is not changed on heating 2 hrs. at 190-200°, on boiling with 0.1 g. NaOH in 15 cc. EtOH and 0.5 cc. H2O, or on acidifying in EtOH with concd. HCl. X in C6H6 or CHCl3, satd. with HCl, gives 81 or 67% of the HCl salt of V. The bond structure of the diamidides are discussed in the light of their ultraviolet absorption spectra.

IT 82208-28-4P, Benzamide, N-(N-phenylbenzimidoyl)-
RL: PREP (Preparation)
(preparation of)

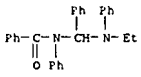
RN 82208-28-4 CAPLUS

L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CN Benzamide, N-[phenyl(phenylamino)methylene]- (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1937:44736 CAPLUS
DOCUMENT NUMBER: 31:44736
ORIGINAL REFERENCE NO.: 31:6223g-i
TITLE: Action of organomagnesium derivatives on the phenylimine derivatives of benzil
AUTHOR(S): Montagne, Marthe; Garry, Marguerite
SOURCE: Compt. rend. (1937), 204, 1659-61
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB On prolonged heating with a large excess of MeMgI, PhC-(:NPh)COPh (I) gives PhCOC(OH) MePh, m. 104.5°, in good yield and PhNH2. With EtMgBr, EtMgI or PhMgBr a similar reaction does not occur but PhNH-COPh (II), BzOH, PhNH2 and Bz2 are formed. [C(:NPh)Ph]2 with MeMgI gives PhCH(NMePh)C-(: NPh) Ph (III), m. 154°, in good yield, and with EtMgI it gives PhCH(NEtPh) C(:NPh)Ph (IV), m. 181°, in poor yield. Besides IV, PhNEt, I and a trace of II are formed. When hydrolyzed with boiling HCl III gives PhNH2 and a HCl salt, m. 145°, which is readily transformed into C6H4.CPh : CPh.NMe, m. 139°. No intermediate α-amino ketone was isolated in the hydrolysis. Hydrolysis of IV gave a small amount of PhNH2 and an unidentified liquid. Only a single active group of I and III reacts with organomagnesium compds.
IT 855271-53-3P, Benzylamine, N-ethyl-N-phenyl-α-N-phenylbenzimido-
RL: PREP (Preparation)
(preparation of)
RN 855271-53-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	79.52	251.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-11.70	-11.70

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